Amendments to the Claims

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims

1. (Currently Amended): A method for selecting at least one lead-candidate compound capable of binding as a ligand to a protein from a ~~compound~~ database of trial compounds comprising information on atomic types and covalent bonds of compounds in the database, comprising:

a) ~~choosing~~ inputting at least one query molecule that is known to bind, or expected to be capable of binding, to the protein; [[and]]

b) ~~selecting~~ screening lead-candidate compounds from the compound database by matching modes of covalent bonds between the query molecule and [a] the trial ~~compound~~ compounds stored in the database and judging similarity of partial structures of the query molecule and the trial ~~compound~~ compounds based on two-dimensional graphs of the query molecule and the trial compounds where each atom is represented as a node and each covalent bond is represented as an arc; and

c) outputting at least one lead-candidate compound capable of binding to the protein.

2-5. (Cancelled)

6. (Currently Amended) The method of claim 1, wherein the compound database comprises information on three-dimensional structures of the trial compounds, and ~~which~~ wherein step (b) further comprises:

[[c)]] estimating a binding scheme of the lead-candidate compounds ~~compound selected in step b)~~ to the protein based on three-dimensional information and binding scheme of the query molecule to the protein ~~of the query molecule~~ and based on correspondence of the partial structures of the query molecule and the ~~trail~~ trial ~~compound~~ compounds;

[[d)]] calculating one or more parameters relating to interaction between the lead-candidate compounds ~~compound~~ and the protein; and

[[e)]] screening the lead-candidate compounds capable of binding as a ligand to the protein based on the parameters relating to interaction between the lead-candidate compounds and the protein ~~calculated in step d)~~.

7. (Currently Amended): The method of claim 1, wherein the compound database comprises information on three-dimensional structures of the trial compounds, and ~~which~~ wherein the step (b) further comprises:

[[c)]] estimating a virtual receptor model which represents physicochemical environment of the ligand binding site of the protein based on information of three-dimensional structures of one or more known ligands capable of binding to the protein;

[[d)]] fitting the lead-candidate compound ~~selected in step b)~~ to the virtual receptor model and judging goodness of fit of the trial compounds to the virtual receptor model; and

[[e)]] screening the ~~trial~~ lead-candidate compounds capable of binding as a ligand to the protein based on the goodness of fit.

8-10. (Cancelled)

11. (Currently Amended) The method of claim 1, ~~further comprising~~ wherein step (a) further comprises constructing the structure of the at least one query molecule by an automatic structure construction method.

12. (Currently Amended) The method of claim 6, ~~further comprising~~ wherein step (a) further comprises constructing the structure of the at least one query molecule by an automatic structure construction method.

13. (Currently Amended) The method of claim 7, ~~further comprising~~ wherein step (a) further comprises constructing the structure of the at least one query molecule by an automatic structure construction method.